(3-Methyl-4-bromophenyl)urea 78508-46-0 | DTXSID10229129

Model Performance

_			
N	Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (75°	Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 1.23e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.31e-01

Confidence level: 6.33e-01

Nearest Neighbors from the Training Set

Image not found

Quinoxalin-5(1H)-one **Measured:** 4.50e-02

Predicted: 9.62e-02

Image not found

Isocil

Measured: 8.70e-03 Predicted: 5.23e-03 Image not found

Bromacil

Measured: 3.12e-03 Predicted: 3.11e-03

Image not found

2-Hydroxy-5-iodopyridine

Measured: 1.81e-02 Predicted: 1.66e-02 Image not found

Tranid

Measured: 8.28e-03 Predicted: 1.40e-02